

Local moment formation in bilayer graphene

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Abstract

The local properties of bilayer graphene (BLG) due to the spatial inhomogeneity of its sublattices are of interest. We apply Anderson impurity model to consider the local moment formation on a magnetic impurity which could be adsorbed on different sublattices of BLG. We find different features for the impurity magnetization when it is adsorbed A and B sublattices. The impurity adsorbed on A sublattice can magnetize even when the impurity level is above the Fermi level and the on-site coulomb energy is very small. But when the impurity is adsorbed on B sublattice the magnetization is possible for limited values of the impurity level and the on-site coulomb energy. This is due to different local density of the low energy states at A and B sublattices which originates from their spatial inhomogeneity. Also we show that electrical controlling the magnetization of adatoms

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besides it's inhomogeneity in BLG allow for possibility of using BLG in spintronic devices with higher potential than graphene.

Keywords: A. Bilayer graphene; D. Anderson impurity model; D. Green's function; D. Local moment.

1 Introduction

Single layer graphene (SLG), a single layer of carbon atoms arranged in a honeycomb lattice, has attracted many experimental and theoretical efforts in the last decade. These efforts result in discovery of many unusual properties[1, 2] which are due to the massless chiral Dirac nature of its charge carriers. One of the attractive topics in SLG is study of the local moment formation on a magnetic impurity adsorbed on a SLG[3, 4, 5, 6, 7]. This is motivated by the use of the scanning tunnelling microscope to control position of an impurity adsorbed on a two-dimensional open surface[8, 9]. Uchoa *et al.* used Anderson model[10] to investigate the necessary conditions for the formation of the local moment on a magnetic impurity adsorbed on a SLG. They found that the impurity adsorbed on SLG magnetizes even when the energy level of the impurity is above the Fermi energy and the on-site coulomb interaction is small. Also they showed that one can control the magnetic moment formation via an external electric field. These behaviors are different from the impurity magnetization in normal metals. This method could be expanded to investigate the impurity magnetization in BLG.

Bilayer graphene (BLG), composed of two layers of graphene with strong interlayer tunnelling, similar to the ordinary two-dimensional electron gas (2DEG) has parabolic band structure. Despite of this similarity, BLG shows unusual properties which are not observed in

2DEG[11, 12]. Due to this feature of BLG, the study of impurity magnetization in BLG can be also attractive. Recently several groups have investigated the possibility of the local moment formation on a magnetic impurity adsorbed on BLG[13, 14, 15]. To scrutinize this topic more, we study it with special emphasis on different features of the local moment formation when the impurity is adsorbed on different sublattices of BLG. We also address the potentiality of BLG doped with the magnetic impurities for spintronics. The paper is organized as follows. The model Hamiltonian and the details of our calculations are presented in the section II. In the section III we discuss our numerical results. Finally we end this paper by summary and conclusions in the section IV.

2 Model Hamiltonian

We apply Anderson model to study the necessary conditions for the local moment formation on an impurity adsorbed on the top of different sublattices of BLG. The total Hamiltonian of a BLG which has adsorbed a magnetic impurity is

$$H_T = H_{BLG} + H_{imp} + H_V, \quad (1)$$

where the Hamiltonian of pure BLG in the nearest neighbor tight-binding approximation is

$$H_{BLG} = -t \sum_{m=1}^2 \sum_{\langle ij \rangle, \sigma} [a_{m\sigma}^\dagger(\mathbf{R}_i) b_{m\sigma}(\mathbf{R}_j) + b_{m\sigma}^\dagger(\mathbf{R}_j) a_{m\sigma}(\mathbf{R}_i)] + \gamma \sum_{i, \sigma} [a_{1\sigma}^\dagger(\mathbf{R}_i) b_{2\sigma}(\mathbf{R}_i) + b_{2\sigma}^\dagger(\mathbf{R}_i) a_{1\sigma}(\mathbf{R}_i)], \quad (2)$$

where $a_{m\sigma}^\dagger(\mathbf{R}_i)$ ($a_{m\sigma}(\mathbf{R}_i)$) creates(annihilates) an electron with spin σ at A sublattice in site i of m -th layer. $t = 2.7$ eV and $\gamma = 0.4$ eV present the nearest neighbor intralayer ($A_1 \longleftrightarrow B_1$ or $A_2 \longleftrightarrow B_2$) and interlayer ($A_1 \longleftrightarrow B_2$) hopping energies respectively. Fig. 1 shows a BLG

lattice. One can diagonalize the momentum dependent Hamiltonian of pure BLG,

$$H_{BLG} = -t \sum_{m=1}^2 \sum_{\mathbf{k}\sigma} [\phi(\mathbf{k}) a_{m\mathbf{k}\sigma}^\dagger b_{m\mathbf{k}\sigma} + \phi^*(\mathbf{k}) b_{m\mathbf{k}\sigma}^\dagger a_{m\mathbf{k}\sigma}] + \gamma \sum_{\mathbf{k}\sigma} [a_{1\mathbf{k}\sigma}^\dagger b_{2\mathbf{k}\sigma} + b_{2\mathbf{k}\sigma}^\dagger a_{1\mathbf{k}\sigma}], \quad (3)$$

to obtain its energy bands which are

$$E_\lambda^\nu = \nu \left(\sqrt{|\phi(\mathbf{k})|^2 + \left(\frac{\gamma}{2}\right)^2} + (-1)^\lambda \frac{\gamma}{2} \right), \quad (4)$$

where $\lambda = 1, 2$ are the energy bands number and $\nu = +(-)$ indicates the conduction(valance) energy bands respectively. $\phi(\mathbf{k}) = \sum_{i=1}^3 e^{i\mathbf{k} \cdot \vec{\delta}_i}$ and $\vec{\delta}_1 = a(\sqrt{3}\hat{x}/2 + \hat{y}/2)$, $\vec{\delta}_2 = a(-\sqrt{3}\hat{x}/2 + \hat{y}/2)$ and $\vec{\delta}_3 = -a\hat{y}$ which are the nearest neighbor vectors. One can expand $|\phi(\mathbf{k})|$ around Dirac points (\mathbf{K} or \mathbf{K}') for $|\mathbf{q}| \ll |\mathbf{K}|$ (where $\mathbf{k} = \mathbf{q} + \mathbf{K}$) to obtain the low energy bands of BLG [1]. In this limit $|\phi(\mathbf{k})| = v_F q$ where $v_F = 3ta/2$ ($\approx 10^6$ m/s) is the Fermi velocity of the Dirac electrons.

The Hamiltonian of the impurity is

$$H_{imp} = \varepsilon_0 \sum_{\sigma} f_{\sigma}^\dagger f_{\sigma} + U n_{\uparrow} n_{\downarrow}, \quad (5)$$

where ε_0 is the energy of the impurity state when it is occupied by one electron and U is the Coulomb energy for double occupancy of the impurity state. $n_{\sigma} = f_{\sigma}^\dagger f_{\sigma}$ is the occupation number and $f_{\sigma}^\dagger (f_{\sigma})$ is the creation (annihilation) operator of an electron with spin σ at the impurity state. Following Anderson[10] we use the mean field approximation to decouple the two-body interaction term as $\sum_{\sigma} \langle n_{-\sigma} \rangle f_{\sigma}^\dagger f_{\sigma} - \langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle$. Hence we can rewrite the Hamiltonian of the impurity as $\sum_{\sigma} \varepsilon_{\sigma} f_{\sigma}^\dagger f_{\sigma}$, where $\varepsilon_{\sigma} = \varepsilon_0 - U \langle n_{-\sigma} \rangle$ is the renormalized energy of the impurity state.

The localized state of the impurity can hybridize with π band of BLG at the adsorb location

via following Hamiltonian

$$H_V = V \sum_{\sigma} (f_{\sigma}^{\dagger} a_{\sigma}(0) + a_{\sigma}^{\dagger}(0) f_{\sigma}). \quad (6)$$

Here the impurity is adsorbed on the A sublattice of site 0 and V is the hybridization strength. Depending on the strength of the hybridization and the on-site coulomb energy, two cases are possible. For the case $n_{\uparrow} \neq n_{\downarrow}$ the local moment forms but for the case $n_{\uparrow} = n_{\downarrow}$ no local local moment. The occupation number of a spin impurity state at zero temperature is given by

$$n_{\sigma} = \int_{-\infty}^{\mu} d\omega \rho_{\sigma}^{imp}(\omega), \quad (7)$$

where $\rho_{\sigma}^{imp}(\omega) = -\frac{1}{\pi} \text{Im} G_{\sigma}^{imp,R}(\omega)$. We use the equation of motion technique to write the retarded Green's function of the impurity, $G_{\sigma}^{imp,R}(\omega)$, as

$$G_{\sigma}^{imp,R}(\omega) = [\omega - \varepsilon_{\sigma} - \Sigma_{imp}^R(\omega) + i0^{+}]^{-1}, \quad (8)$$

in which the retarded self-energy of the impurity is

$$\Sigma_{imp}^R(\omega) = V^2 G_{\alpha\alpha,\sigma}^{0R}(\omega) = \frac{V^2}{\sqrt{N}} \sum_{\mathbf{q}} G_{\alpha\alpha,\sigma}^{0R}(\mathbf{q}, \omega), \quad (9)$$

where $\alpha = A$ ($\alpha = B$) when the impurity is adsorbed on A (B) sublattice of BLG and $G_{\alpha\alpha,\sigma}^{0R}(\mathbf{q}, \omega)$ is the clean Green's function of BLG at α sublattice. After integration over momentum we found the Green's functions as

$$\begin{aligned} G_{AA,\sigma}^{0R}(\omega) = & -\frac{1}{2D^2} [\omega \ln \left| \frac{(\omega - \gamma/2)^2 - D^2}{\omega(\omega - \gamma)} \right| + \omega \ln \left| \frac{(\omega + \gamma/2)^2 - D^2}{\omega(\omega + \gamma)} \right|] \\ & -i \frac{\pi}{2D^2} [|\omega| \theta(\gamma - |\omega|) + 2|\omega| \theta(|\omega| - \gamma)] \theta(|\omega| - D), \end{aligned} \quad (10)$$

and

$$\begin{aligned} G_{BB,\sigma}^{0R}(\omega) = & -\frac{1}{2D^2} [(\omega - \gamma) \ln \left| \frac{(\omega - \gamma/2)^2 - D^2}{\omega(\omega - \gamma)} \right| + (\omega + \gamma) \ln \left| \frac{(\omega + \gamma/2)^2 - D^2}{\omega(\omega + \gamma)} \right|] \\ & -i \frac{\pi}{2D^2} [(|\omega| + \gamma) \theta(\gamma - |\omega|) + 2|\omega| \theta(|\omega| - \gamma)] \theta(|\omega| - D), \end{aligned} \quad (11)$$

where D is the high-energy cutoff of BLG bandwidth and $\theta(x)$ is the step function. Eqs. (7)-(11) construct a closed set of equations which should be solved selfconsistently to obtain the occupation number. Our numerical results are presented in the next section.

3 Numerical Results

The local magnetic moment exists when the occupation number of two spins at the impurity level are different, namely whenever $n_{\uparrow} \neq n_{\downarrow}$. The occupation number for a giving spin, n_{σ} , can be calculated self-consistently from Eqs. (7)-(11). We use following dimensionless parameters, $x = \Delta D/U$ and $y = (\mu - \varepsilon_0)/U$ with $\Delta = \pi V^2/D^2$, in the reminder of this paper.

Fig. 2 presents our results for the curves of the boundary separating the magnetic and non-magnetic phase of the impurity state. These curves are corresponding to different values of the interlayer tunnelling energies, $\gamma = 0$, $\gamma = 0.175$ eV and $\gamma = 0.4$ eV, when the impurity is adsorbed on A sublattice (left panel) or on B sublattice (right panel). The other parameters are $\varepsilon_0 = 0.2$ eV, $V = 1.0$ eV and $D \approx 7$ eV. We considered all possible locations for the impurity adsorption on BLG sublattices. Our results for BLG case when the impurity is adsorbed on B sublattice and for SLG limit ($\gamma = 0$) are in agreement with previous works[3, 13]. Also we see that by increasing the interlayer tunnelling energy (transforming from two separated SLG to BLG case) for the impurity adsorbed on A sublattice the size of the magnetic region increases while when the impurity is adsorbed on B sublattice it decreases. Note that the local density of states (LDOS) at A and B sublattices of BLG[16] are

$$N_A(\omega) = \frac{1}{2D^2} [|\omega|\theta(\gamma - |\omega|) + 2|\omega|\theta(|\omega| - \gamma)]\theta(|\omega| - D), \quad (12)$$

and

$$N_B(\omega) = \frac{1}{2D^2}[(|\omega| + \gamma)\theta(\gamma - |\omega|) + 2|\omega|\theta(|\omega| - \gamma)]\theta(|\omega| - D), \quad (13)$$

respectively. We see that by increasing the interlayer tunnelling energy, the local density of the low energy states at A sublattice decreases, so the hybridization of the impurity level with carbon atom located at A sublattice becomes weaker with respect to that in SLG. This leads to easier formation of the localized magnetic moment on the impurity adsorbed on A sublattice. So the size of the magnetic region increases. But for the impurity adsorbed on B sublattice, increasing the interlayer tunnelling energy increases the local density of the low energy states. This leads to enhancement of the hybridization with impurity state. So the magnetic moment formation region decreases.

Furthermore when the impurity is adsorbed on A sublattice, the magnetic boundary crosses the line $y = 0$. This is due to the large broadening of the impurity level, as the local moment can form even when ε_0 is above the Fermi energy. But when the impurity is adsorbed on B sublattice this feature disappears approximately. This could be explained by the small broadening of impurity level which is due to the nonzero amount of the LDOS at around the impurity level.

Fig. 3 shows effects of ε_0 and V variation on the size of the magnetic region. We see that as $\varepsilon_0 \rightarrow 0$ the local moment formation becomes more possible so the size of the magnetic region grows (for impurities adsorbed on both A and B sublattices). This can be explained by this fact that the LDOS around the impurity level is suppressed which allows for easy formation of the local moment. Furthermore when the impurity is adsorbed on A sublattice the size of the magnetic region increases more, because at low energy states, $\omega \rightarrow 0$, the LDOS on A sublattice

decreases faster than that on B sublattice. Also as we expect, by increasing the hybridization strength the size of the magnetic region decreases.

Similar to SLG, in the BLG the magnetization of the impurity can be controlled by applying an electric field via a back gate which can change the chemical potential. This allows for the potentiality of BLG for spintronics. This can be clarified by considering the chemical potential dependence of the occupation number and susceptibility of the magnetic impurity. The magnetic susceptibility of the impurity is defined as $\chi = \mu_B \sum_{\sigma} \sigma (dn_{\sigma}/dB)_{B=0}$ in the zero magnetic field limit. This can be rewritten as

$$\chi = -\mu_B^2 \sum_{\sigma} \frac{d\langle n_{\sigma} \rangle}{d\varepsilon_{\sigma}} \frac{1 - U \frac{d\langle n_{-\sigma} \rangle}{d\varepsilon_{-\sigma}}}{1 - U^2 \frac{d\langle n_{-\sigma} \rangle}{d\varepsilon_{-\sigma}} \frac{d\langle n_{\sigma} \rangle}{d\varepsilon_{\sigma}}}, \quad (14)$$

where $\varepsilon_{\sigma} = \varepsilon_0 - \sigma\mu_B B + Un_{-\sigma}$ is the energy of the impurity spin state in the presence of the magnetic field which tends to zero. The impurity magnetizes when a bubble shape exists in the occupation number curve. At the edges of this magnetic bubble the corresponding susceptibility has two peaks which show the strength of the magnetic transition.

In Fig. 4 we plotted $n_{\sigma}(\mu)$ and $\chi(\mu)$ of a magnetic impurity adsorbed on A sublattice (left panels) and B sublattice (right panels) for different values of the on-site coulomb energies, $U = 96$ meV (dotted-dashed curves), $U = 48$ meV (dashed curves) and $U = 24$ meV (solid curves). The other parameters are considered as $\varepsilon_0 = 0.2$ eV, $V = 1$ eV and $\gamma = 0.4$ eV. We see that one can control amount of the local moment of the magnetic impurity adsorbed on both A and B sublattices via varying the chemical potential. Furthermore Figs. 4 shows that controlling the local magnetic moment on A sublattice is possible for wide range of the on-site coulomb energies.

It has been reported in the recent considerations that the magnetic coupling between magnetic moment of adatoms adsorbed on same (different) sublattices is ferromagnetic (antiferromagnetic) in both single layer graphene (SLG) [18] and bilayer graphene (BLG) [19, 20]. Furthermore we showed that the local moment strengths of magnetic adatoms on different sublattices of BLG are not equal. Hence in BLG even when magnetic adatoms are distributed randomly on different sublattices we have net local moment. While in SLG, because the local moment strengths of magnetic adatoms adsorbed on different sublattices are equal[18], for random distribution of magnetic adatoms there is not net local moment. These features allow for using BLG as spin switcher in the spintronics devices with higher potential than SLG.

This figure also sustains our previous results about more possibility of the impurity magnetization on A sublattice in contrast to B sublattice. For the impurity adsorbed on A sublattice with mentioned parameters, at a small on-site coulomb energy about $U = 96$ meV a strong magnetic moment of $\sim 0.8\mu_B$ forms in the entire magnetic region approximately. By decreasing the on-site coulomb energy, size of the magnetic region decreases and the magnetic transition phase becomes very sharp (Fig. 4(a) and 4(b)), but even at $U = 24$ meV a local magnetic moment of $\sim 0.3\mu_B$ forms. The impurity magnetization for a such small on-site coulomb energy neither in normal metal [17] nor in SLG [3] has not been reported. While when the impurity is adsorbed on B sublattice the impurity magnetization is possible for on-site coulomb energies which are nearly thrice larger. Also we see that by decreasing U the size of the magnetic bubble rapidly diminishes.

4 Summary and conclusions

In summary, we considered the local magnetic moment formation of a magnetic impurity adsorbed on a BLG. We found different features for the magnetization of the impurity adsorbed on A and B sublattices.

We showed that the magnetic impurity adsorbed on A sublattice can magnetize even at very small on-site coulomb energies. This is not reported neither in normal metal [17] nor in SLG [3]. This is due to the very low LDOS at A sublattice that decreases the effect of the hybridization with the impurity level and allow for easy formation of the local moment. Also we found that the local moment forms even when the energy of bare impurity level is above the Fermi energy. This can be explained by large broadening of the impurity level.

But when the impurity is adsorbed on B sublattice, due to the large local density at low energy states the hybridization with the impurity level is enhanced. This limits the impurity magnetization on B sublattice in comparison with that on A sublattice of BLG and also with that on all sublattices of SLG. Also due to the small broadening of the impurity level, the impurity magnetizes approximately only when the bare impurity level is below the Fermi energy.

Finally we showed that by varying the chemical potential via an external electric field one can control the local moment of the magnetic impurity adsorbed on both A and B sublattices. This feature besides inhomogeneity of the adatom's magnetization in BLG allow for using BLG as spin switcher in spintronics devices.

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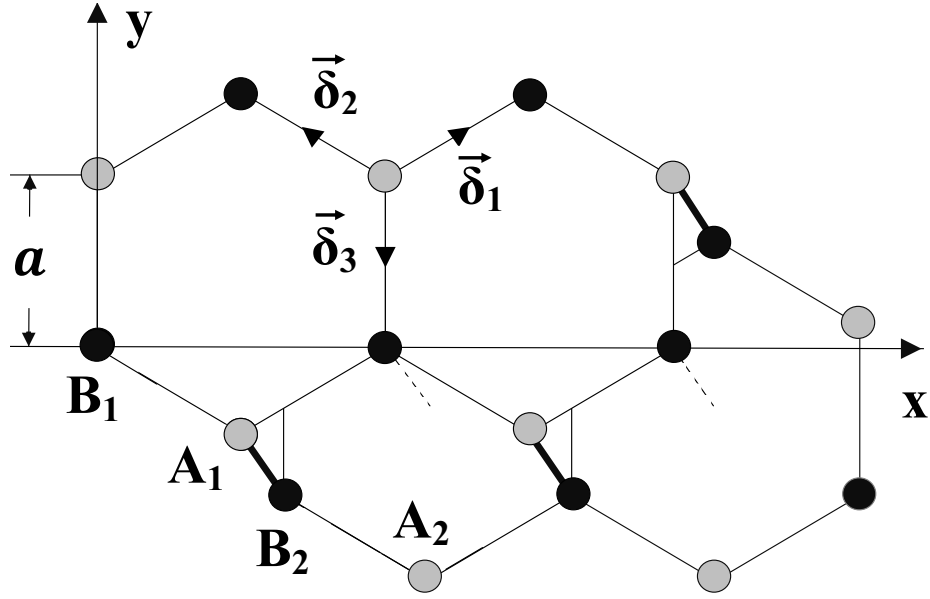


Figure 1: Lattice structure of BLG. $\vec{\delta}_1 = a(\sqrt{3}\hat{x}/2 + \hat{y}/2)$, $\vec{\delta}_2 = a(-\sqrt{3}\hat{x}/2 + \hat{y}/2)$ and $\vec{\delta}_3 = -a\hat{y}$ are three vectors that are drawn from connects A_1 sublattice to it's nearest neighbors.

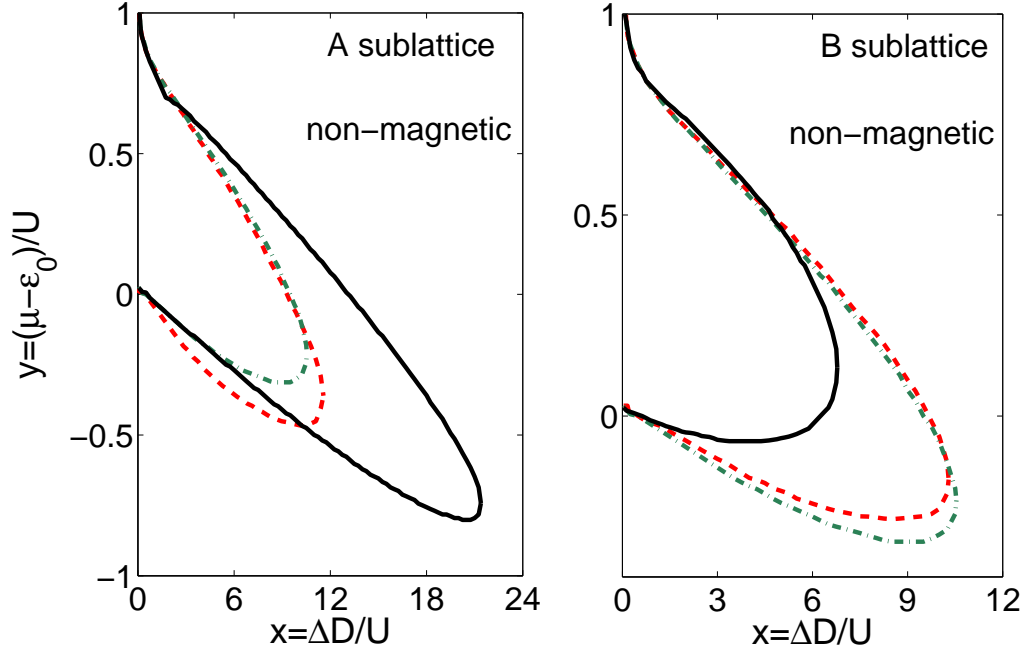


Figure 2: The boundary between magnetic and non-magnetic states of an impurity adsorbed on A sublattice (Left panel) and B sublattice (Right panel) in a bilayer graphene lattice for different interlayer hopping, $\gamma_1 = 0.4$ (Solid curves), $\gamma_1 = 0.185 eV$ (dashed curves) and $\gamma_1 = 0.0 eV$ (dotted-dashed curves). The other parameters are $\varepsilon_0 = 0.2 eV$, $V = 1 eV$.

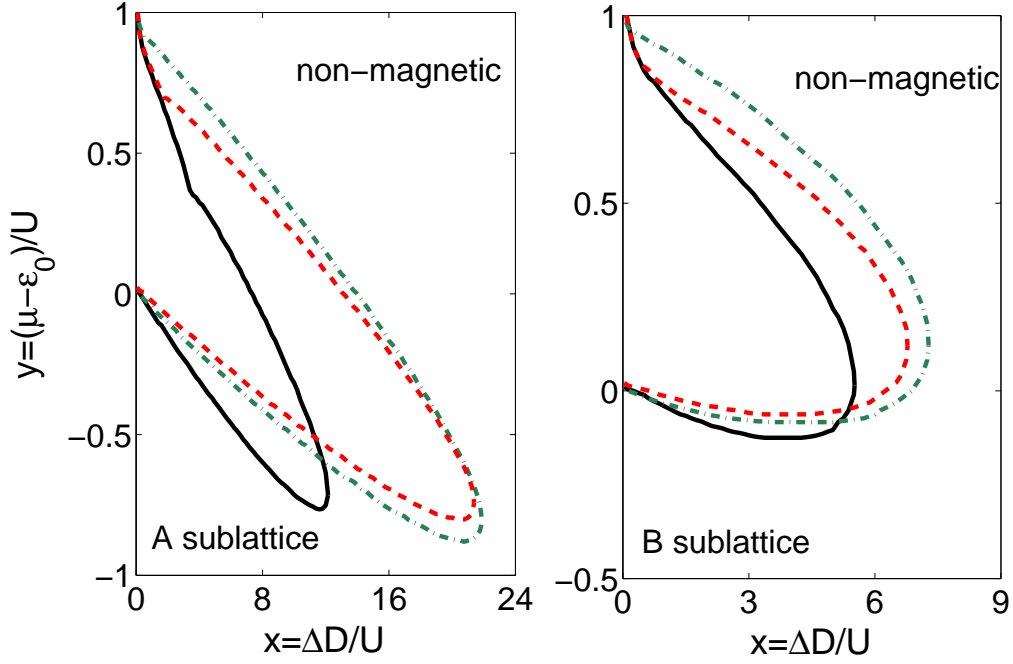


Figure 3: The boundary between magnetic and non-magnetic states of an impurity adsorbed on A sublattice (Left panel) and B sublattice (Right panel) in a bilayer graphene lattice with $\gamma = 0.4eV$. Solid curves: $\varepsilon_0 = 0.35eV$, $V = 1eV$; dashed curves: $\varepsilon_0 = 0.2eV$, $V = 1eV$; dotted-dashed: $\varepsilon_0 = 0.2eV$, $V = 0.5eV$.

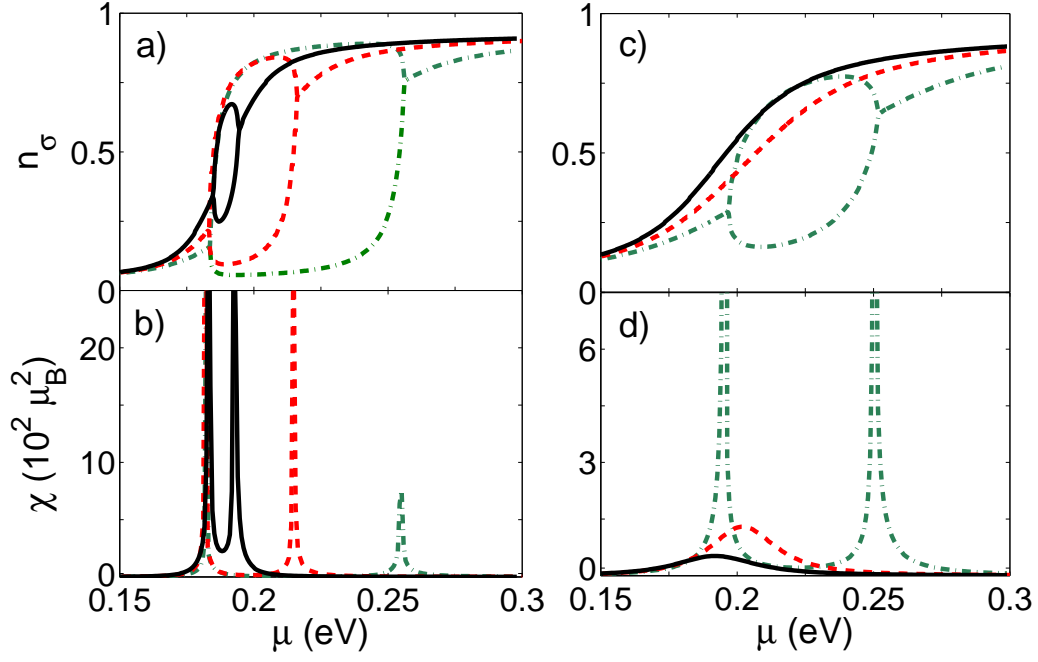


Figure 4: $n_\sigma(\mu)$ and $\chi(\mu)$ curves of an magnetic impurity with $\varepsilon_0 = 0.2eV$ and $V = 1eV$ adsorbed on A sublattice (left panels) and B sublattice (right panels). Dotted-dashed: $U = 0.096eV$; dashed curves: $U = 0.048eV$; solid curves: $U = 0.024eV$.